

Contact transformations and the quantisation of constraint systems

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The possibility of quantizing a constraint system, in such a way as to respect coordinate transformations in the configuration space, is explored. It is found that, within the Schrödinger representation, covariance of the quantum theory can be maintained only under those contact transformations leaving the Lagrange multiplier unchanged (within a constant scaling).

1. Introduction

It is well known that the Euler-Lagrange equations for a classical system of finite degrees of freedom are covariant under a general coordinate transformation in configuration space: if the equations are valid in one coordinate system they are valid in any other; this holds both for regular as well as for singular systems (see e.g. ref. [1]).

The question naturally arises whether this covariance can be maintained at the quantum level. We intend to investigate this problem for lagrangians, that are quadratic in the velocities.

In the case of a regular system the answer to the above question is positive: one has just to select for the corresponding hamiltonian (quadratic in the momenta) the Laplace-Beltrami operator plus a possible multiple of the Ricci scalar [2].

In the presence of constraints, since the configuration space contains the Lagrange multipliers, the situation radically changes. As we shall see, it is not possible to maintain the covariance of the corresponding quantum theory under contact transformations involving all the coordinates of configuration space; this holds, no matter which hermitian factor ordering one selects.

2. Contact transformations versus quantum theory

Let us consider the lagrangian

$$\mathcal{L} = \frac{1}{2} \gamma_{\mu\nu}(q) \dot{q}^\mu \dot{q}^\nu - V(q),$$

where $\det \gamma \neq 0$.

The Euler-Lagrange equations can be viewed as derived geodesic equations on the manifold with metric $\gamma_{\mu\nu}$ (with driving force $-\partial V/\partial q^\mu$), and are therefore covariant under a contact transformation (CT). The corresponding hamiltonian is

$$H = \frac{1}{2} \gamma^{\mu\nu} P_\mu P_\nu + V(q),$$

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with $\gamma^{\mu\nu}$ the inverse of $\gamma_{\mu\nu}$.

The operator

$$\hat{H} = -\frac{1}{2} \nabla + V(d) + kR$$

(where ∇ stands for the laplacian and R is the Ricci scalar constructed from $\gamma_{\mu\nu}$) is covariant under a CT. This means that if one effects the change of coordinates $q^\mu \rightarrow \tilde{q}^\mu = f^\mu(q)$, as the potential V and the wavefunction Ψ are scalars, one will have

$$\hat{H}\Psi := -\frac{1}{2} \nabla \Psi + V(\tilde{q}) \Psi + k\tilde{R}\Psi = -\frac{1}{2} \nabla \Psi - V(q) \Psi + kR\Psi = \hat{H}\Psi.$$

Let us now turn to the singular action

$$\mathcal{S} = \int \left(\frac{1}{2N} \gamma_{\mu\nu} \dot{q}^\mu \dot{q}^\nu - NV(q) \right) dt, \quad \mu = 1, 2, \dots, d,$$

with $\det \gamma \neq 0$.

This is a generalization of various reduced actions appearing in quantum cosmology [3]. The lagrangian corresponding to (5) has a primary first class constraint

$$X_1 := P_N \approx 0. \quad (6)$$

The canonical hamiltonian reads

$$H_c = N [\frac{1}{2} \gamma^{\mu\nu} P_\mu P_\nu + V(q)].$$

The constraint $X_1 \approx 0$ must be preserved in time; therefore

$$0 \approx \dot{X}_1 \approx \{ X_1, H_c \} + \lambda \{ X_1, X_2 \} \rightarrow \{ X_1, H_c \} \approx 0 \rightarrow X_2 := \frac{1}{2} \gamma^{\mu\nu} P_\mu P_\nu + V(q) \approx 0. \quad (7)$$

At this stage the Dirac-Bergmann algorithm is terminated since $\{ X_2, H_c \} = 0$ and $\{ X_2, X_1 \} = 0$. The constraints (6) and (7) are first class.

Under a general CT, $(q, N) \rightarrow (\tilde{q}, \tilde{N})$ the classical equations of motion are covariant in the sense that their validity in the (\tilde{q}, \tilde{N}) coordinate system implies their validity in the original coordinate system and vice versa. According to Dirac's proposal [4], in quantizing system (5) one must realize constraints (6) and (7) as hermitian operators under some measure $\mu(q, N)$ and the quantum states $\Psi(q, N)$ as their null eigenvectors.

Using the Schrödinger representation

$$\hat{q}^\mu = q^\mu, \quad \hat{N} = N, \quad \hat{P}_\mu = -i\partial_\mu, \quad \hat{P}_N = -i\partial/N,$$

one can write the hermitian operator corresponding to (6) as

$$\lambda_1 = \frac{1}{2\mu} (\mu \hat{P}_N + \hat{P}_N \mu). \quad (8a)$$

The hermitian operator quadratric in momenta corresponding to (7) is

$$\lambda_2 = \frac{1}{2\mu} \hat{P}_\mu \gamma^{\mu\nu} \mu \hat{P}_\nu + B + V(q), \quad (8b)$$

where B is an arbitrary (real) function of q constructed from: $\gamma_{\mu\nu}, \gamma_{\mu\nu\rho}, \gamma_{\mu\nu\rho\sigma}, \gamma_{\mu\nu\rho\sigma\tau}$ quadratic in first and linear in second derivatives of $\gamma_{\mu\nu}$. The appearance of B is a quantum ordering effect resulting from an ordering in which a function of $q^{\mu\nu}(q)$ stands to the far right; thus B is of order \hbar^2 . As we shall later see, B is nothing but a linear function of R , just like in the case of a regular system (see relation (3)).

The states Ψ obey the differential equations

$$\hat{X}_1 \Psi = 0, \quad \hat{X}_2 \Psi = 0. \quad (9a, b)$$

Eq. (9a) reads

$$\mu \frac{\partial \Psi}{\partial N} + \frac{1}{2} \Psi \frac{\partial \mu}{\partial N} = 0,$$

yielding as its general solution

$$\Psi(\tilde{q}, N) = \mu^{-1/2} \Phi(q).$$

Returning to the classical system described by action (5) we see that the most general CT preserving the character of N as a Lagrange multiplier is of the form

$$\left[\begin{array}{c} q^\mu \\ N \end{array} \right] \rightarrow \left[\begin{array}{c} \tilde{q}^\mu = g^\mu(q) \\ \tilde{N} = \exp[f(q)]N \end{array} \right].$$

Under this transformation, the action (5) must be a scalar; thus yielding the lagrangian in the new coordinates:

$$L = \frac{\exp[f(q)]}{2N} \gamma_{\mu\nu} \frac{\partial q^\mu}{\partial \tilde{q}^\beta} \frac{\partial q^\nu}{\partial \tilde{q}^\alpha} \dot{q}^\alpha \dot{q}^\beta - \frac{\nu(q)}{\exp[f(q)]} \tilde{N} = \frac{1}{2\tilde{N}} \tilde{\gamma}_{\mu\nu} \dot{\tilde{q}}^\mu \dot{\tilde{q}}^\nu - \tilde{V}(\tilde{q}) \tilde{N}. \quad (12)$$

If we keep q unchanged, i.e.,

$$\left[\begin{array}{c} q^\mu = q^\mu \\ N = \exp[f(q)]N \end{array} \right], \quad (13)$$

then the transformation induced on the metric $\gamma_{\mu\nu}$ is similar to a conformal transformation in the submanifold with coordinates q^μ and metric tensor $\gamma_{\mu\nu}$; one must however keep in mind that this transformation is in fact a coordinate transformation in the configuration space with coordinates (q^μ, N) .

In the special case of (13) eq. (12) becomes

$$L = \frac{1}{2\tilde{N}} \exp[f(q)] \gamma_{\mu\nu}(q) \dot{q}^\mu \dot{q}^\nu - \frac{\nu(q)}{\exp[f(q)]} \tilde{N}. \quad (14)$$

The Dirac-Bergmann algorithm for (12) yields the constraints

$$\tilde{\lambda}_1 = \tilde{P}_\mu \approx 0, \quad \tilde{\lambda}_2 = \frac{1}{2} \tilde{\mu}_{\mu\nu} \tilde{P}_\mu \tilde{P}_\nu + \tilde{V}(\tilde{q}) \approx 0.$$

The quantum analogues of $\tilde{\lambda}_1, \tilde{\lambda}_2$ are

$$\tilde{\lambda}_1 = \frac{1}{2\tilde{\mu}} (\tilde{\mu} \tilde{P}_\mu + \tilde{P}_\mu \tilde{\mu}), \quad \tilde{\lambda}_2 = \frac{1}{2\tilde{\mu}} \tilde{\mu}_{\mu\nu} \tilde{\mu}^{\mu\nu} \tilde{P}_\mu + \tilde{V}(\tilde{q}) + \tilde{B}.$$

In these coordinates the states $\Psi(\tilde{q}, \tilde{N})$ obey the differential equations

$$\tilde{\mu}(\tilde{q}, \tilde{N}) \tilde{d}\tilde{q} d\tilde{N} = \mu(q, N) dq dN \Psi(q, N).$$

If one wants the quantum theories in (q, N) and (\tilde{q}, \tilde{N}) to be equivalent one has to require the following:

Requirement (a). The inner product in the Hilbert space must be scalar under the transformation (11), i.e.,

$$(16a)$$

$$\tilde{\mu}(\tilde{q}, \tilde{N}) \tilde{d}\tilde{q} d\tilde{N} = \mu(q, N) dq dN \Psi(q, N).$$

Requirement (b). The states should also be scalars:

$$\Psi(\tilde{q}, \tilde{N}) = \Psi(q, N).$$

One should in fact allow for a phase $\exp[i\theta(q, N)]$ in this transformation, i.e., $\Psi(\tilde{q}, \tilde{N}) = \exp[i\theta(q, N)] \Psi(q, N)$.

However, as it is shown in the discussion θ turns out to be a constant.

To this end, let us accept transformation (22) for the wave function. Then eq. (16a) reads

$$(16b)$$

$$\Psi(\tilde{q}, \tilde{N}) = \exp[W(q, N)] \Psi(q, N),$$

$$(16c)$$

$$W(q, N) = \int f_\mu(q) dq.$$

$$(16d)$$

$$W(q, N) = \int f_\mu(q) dq.$$

Requirement (c). The system of equations (16) expressed in (q, N) coordinates must be equivalent to system (9).

In the special case of a transformation keeping N fixed, i.e.,

$$\left[\begin{array}{c} q^\mu \\ N \end{array} \right] \rightarrow \left[\begin{array}{c} \tilde{q}^\mu = g^\mu(q) \\ \tilde{N} = N \end{array} \right], \quad (18)$$

all requirements (a), (b), (c) above can be satisfied with a choice analogous to (3) for $\tilde{\lambda}_2$. Then the linear operator reads

$$\tilde{\lambda}_1 = \frac{1}{2\tilde{\mu}} (\tilde{\mu} \tilde{P}_N + \tilde{P}_N \tilde{\mu}) = \frac{1}{2\mu J(q)} [J(q)\mu \tilde{P}_N + \tilde{P}_N J(q)\mu] = \tilde{\lambda}_1,$$

where $J(q) = |\partial q / \partial \tilde{q}|$. Since a transformation of the form (11) can be viewed as a composition of a transformation of the form (18) followed by one of the form (13), the investigation will, from now on, be limited to transformations of the form (13).

Under such a transformation the momenta $\tilde{p}_\mu, \tilde{P}_N$ and the measure transform as follows:

$$\tilde{p}_\mu = \tilde{P}_\mu - f_\mu N \tilde{P}_N, \quad \tilde{P}_N = \exp(-J) \tilde{P}_N, \quad \tilde{\mu} = \exp(-J) \mu. \quad (19a, b, c)$$

The operator given in (15a) translated in the (q, N) coordinates reads

$$\tilde{\lambda}_1 = \frac{1}{2\tilde{\mu}} (\tilde{\mu} \tilde{P}_N + \tilde{P}_N \tilde{\mu}) = \exp(-J) \tilde{\lambda}_1. \quad (20)$$

This shows that (16a) is equivalent to (9a).

The quadratic term of $\tilde{\lambda}_2$ in (15b) acting on $\Psi(\tilde{q}, \tilde{N}) = \Psi(q, N)$ and translated in the (q, N) variables is

$$\frac{1}{2\tilde{\mu}} \tilde{\mu}_{\mu\nu} \tilde{\mu}^{\mu\nu} \tilde{P}_\mu \tilde{P}_\nu = \exp(-J) \frac{1}{2\mu} \mu_{\mu\nu} \mu^{\mu\nu} P_\mu P_\nu + \frac{\exp(J)}{2\mu} [P_\mu \exp(-2J) \mu^{\mu\nu} \mu^{1/2} P_\nu \phi + T \psi], \quad (21)$$

where T contains first and second derivatives of ϕ and μ and first derivatives of $\gamma_{\mu\nu}$ (for its explicit form see (24) below with $W=0$).

In order for (16b) to be equivalent to (9b), since B does not contain derivatives of ϕ , the terms proportional to $P_\mu \phi$ must vanish, i.e.,

$$[P_\mu \exp(-2J)]_1 = 0 = f_\mu = 0 \Rightarrow f = \text{constant}.$$

This fact shows that requirements (a), (b), (c) can be satisfied if and only if one is restricted to transformations analogous to (18): $(q^\mu, N) \rightarrow (\tilde{q}^\mu(q), cN)$ where c a constant.

Nevertheless, because of the apparent similarity of a conformal transformation to the change induced in the metric tensor $\gamma_{\mu\nu}$ by a CT of the form (13), some authors [5] allow the transformation of the wavefunction to be of the form

$$\tilde{\Psi}(\tilde{q}, \tilde{N}) = \exp[W(q, N)] \Psi(q, N),$$

where W is a real function.

If this transformation is allowed, then f_μ is not zero in general, and the contact transformation is not restricted to just the scale N by a constant.

Indeed, taking $B = -(d-2)R/8(d-1)$, $\mu = \sqrt{f}$ and $W = -(d-2)f/2$ these authors obtain the covariance of the $\tilde{\lambda}_1, \tilde{\lambda}_2$, thus satisfying requirement (c). However requirements (a) and (b) are not satisfied.

It is interesting to investigate if there is another choice of B, μ and W satisfying requirements (a) and (c).

To this end, let us accept transformation (22) for the wave function. Then eq. (16a) reads

$$\Psi(\tilde{q}, \tilde{N}) = \Psi(q, N).$$

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$\hat{X}_1 \Psi = 0 \leftrightarrow \exp(-J) \hat{X}_1 \exp(w) \Psi = 0 \leftrightarrow W = W(q)$,
while eq. (16b) becomes

$$\begin{aligned} & \frac{1}{2\mu} \exp(w) P_\mu \gamma^\mu P_\nu \Psi + \tilde{B} \exp(w) \Psi + \tilde{V} \exp(w) \Psi \\ & + \frac{1}{2\mu} \{ 2 \exp(-J) [\hat{\beta}_\mu, \exp(w)] \gamma^{\mu\nu} \mu^{1/2} + \exp(J) [\hat{\beta}_\mu, \exp(-2J)] \gamma^{\mu\nu} \mu^{1/2} \exp(w) \} \hat{\beta}_\nu \Phi \\ & + \frac{\exp(-J)}{2} \mu^{1/2} [\hat{\beta}_\mu, \exp(w)] \gamma^{\mu\nu} \mu^{-1/2} \Psi + \frac{\exp(-J)}{2\mu} \mu^{1/2} [\hat{\beta}_\mu, \gamma^{\mu\nu} \mu^{1/2} [\hat{\beta}_\nu, \exp(w)]] \Phi \\ & + \frac{\exp(J)}{2\mu} \mu^{3/2} \gamma^{\mu\nu} [\hat{\beta}_\mu, \exp(-2J)] [\hat{\beta}_\nu, \exp(w) \mu^{-1/2}] \Psi \\ & - \frac{\exp(J)}{2\mu} \mu^{1/2} N [\hat{\beta}_\mu, \exp(-2J) \gamma^{\mu\nu} \mu \hat{\beta}_\nu \exp(w) [\hat{\beta}_{N\mu} \mu^{-1/2}]] \Psi \\ & - \frac{\exp(-J)}{2\mu} f_{\mu\nu} N \gamma^{\mu\nu} \mu^{1/2} [\hat{\beta}_{N\mu} \mu [\hat{\beta}_{N\nu} \exp(w) \mu^{-1/2}]] \Psi \\ & - \frac{\exp(-J)}{2\mu} \exp(w) \mu^{3/2} N^2 \gamma^{\mu\nu} f_{\mu\nu} [\hat{\beta}_{N\mu} [\hat{\beta}_{N\nu} \mu^{-1/2}]] \Psi \\ & + \frac{\exp(-J)}{2\mu} \exp(w) N \mu^{1/2} \gamma^{\mu\nu} f_{\mu\nu} f_{\nu\lambda} [\hat{\beta}_{N\mu} \mu N] [\hat{\beta}_{N\lambda} \mu^{-1/2}] \Psi = 0 \end{aligned} \quad (24)$$

Again requirement (c) implies that the terms proportional to $\hat{\beta}_\mu \Phi$ in (24) should vanish.
 $\gamma^{\mu\nu} W_\mu = \gamma^{\mu\nu} f_{\mu\nu} \leftrightarrow W = f + \text{constant}$.

The only measure $\mu(q, N)$ (constructed out of $\gamma_{\mu\nu}$ and N) satisfying requirement (a) under a CT of the form (18) is

$$\mu(q, N) = \gamma^{1/2} h(N).$$

With this measure the quadratic term of \hat{X}_2 is exactly the laplacian. In order to satisfy requirement (c) the term B should transform as a scalar. The only available scalar, which is linear in the second derivatives of $\gamma_{\mu\nu}$, is the Ricci scalar; thus one must put $B(N) = \phi(N)R$.

If $\mu(q, N)$ is to satisfy requirement (a) under the general CT (11) it must be
 $\mu(q, N) = \gamma^{1/2} N^a$ with $a = -(d+2)/2$.

For this choice of μ and B eq. (24) reads

$$\frac{1}{2\mu} \hat{\beta}_\mu \gamma^{\mu\nu} \mu \hat{\beta}_\nu \Psi + \frac{(d-2)^2}{32} f_{\mu\nu} \gamma^{\mu\nu} \Psi - \frac{(d-2)}{8} (\nabla) \Psi + \varphi(N) \tilde{R} \exp(J) \Psi + \tilde{V} \exp(J) \Psi = 0. \quad (27)$$

Under transformation (13) the Ricci scalar corresponding to $\gamma_{\mu\nu}$ transforms as

$$\tilde{R} = \exp(-J) \left(R + (d-1) \nabla J + \frac{(d-2)(d-1)}{4} \gamma^{\mu\nu} f_{\mu\nu} \right). \quad (28)$$

Using this in eq. (27) one obtains

$$\begin{aligned} & \frac{1}{2\mu} \hat{\beta}_\mu \gamma^{\mu\nu} \hat{\beta}_\nu \Psi + \varphi(N) R \Psi + V(q) \Psi + \left(\frac{d-2}{8} + \varphi(N)(d-1) \right) (\nabla) \Psi \\ & + \frac{d-2}{4} \left(\frac{d-2}{8} + \varphi(N)(d-1) \right) \gamma^{\mu\nu} f_{\mu\nu} \Psi = 0. \end{aligned}$$

Thus requirement (c) implies $\varphi(N) = -(d-2)/8(d-1)$.
With this choice of W and B one has

$$\hat{X}_2 \Psi = \hat{X}_2 \Psi.$$

The final form of \hat{X}_2 is

$$\hat{X}_2 = -\frac{1}{2\sqrt{\gamma}} \partial_\mu \gamma^{\mu\nu} \sqrt{\gamma} \partial_\nu - \frac{d-2}{8(d-1)} R + V(q).$$

3. Discussion

We have investigated the problem of whether, for a constraint system, the covariance under contact transformations can be maintained at the quantum level. We have found that, if one accepts the transformation of the wavefunction to be that of a scalar (requirement (b)), then the transformations which are covariances of the quantum theory are only those described by eq. (18) plus a constant scaling of N . This results holds true even if one allows a phase factor $\exp(i\theta(q, N))$ in the transformation of the wavefunction. Imposing requirement (c) one obtains eqs. (23), (25) with $W(q, N)$ substituted by $i\theta(q, N)$, i.e.,

$$\theta(q, N) = \theta(q), \quad i\theta(q) = f(q) + C_1 + iC_2, \quad \theta(q) = C_1, \quad f(q) = C_2.$$

In imposing requirement (b) we have of course accepted that Ψ is a function of q and N . This is an unavoidable when one intends to quantize a constraint system à la Dirac: The first class constraints, which are to be realized as conditions on the quantum states, are generators of gauge symmetries; thus the state vectors will, in principle, be functions of all configuration variables, dynamical and gauge as well. The same reasoning applies for the measure appearing in requirement (a). Despite this, one can see that the probability density $\mu|\Psi|^2$ does not depend on N ($|\mu|\Psi|^2 = \mu|\mu^{-1/2}\Phi|^{2m} |\Phi|^2$).

We have also seen that if one is willing to abandon requirement (b), then it is possible to satisfy requirement (c) or requirement (c) and requirement (a) with suitable choices of W and B (in (8b)).

However, it is our opinion that requirement (b) should not be abandoned: The origin of the freedom to arbitrarily rescale the quadratic constraint lies in performing the coordinate transformation (13) and not in a "gauge" transformation of $\gamma_{\mu\nu}$ and Ψ ($\gamma_{\mu\nu} \rightarrow \exp(U) \gamma_{\mu\nu}, \Psi \rightarrow \exp(V) \Psi$). Consequently there is no reason whatsoever to accept transformation (22) for the wavefunction and abandon requirement (b).

Finally, it is interesting to remark that the situation described above is reminiscent of the noncommutativity of canonical transformations with the quantization procedure: Contact transformations involving the Lagrange multiplier N do not commute with the quantum theory.

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Estimation of the central charge by Monte Carlo simulations

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Using an idea put forward by J.L. Cardy, we demonstrate how to obtain a good estimate for the central charge c of a conformally invariant field theory by Monte Carlo simulations of the corresponding statistical model away from criticality, but in the scaling region; the two-dimensional three-state Potts model in a magnetic field is used as a test case. Determining c in this way is feasible because of a big increase in the availability of computational power and because of the invention of stochastic cluster algorithms, which allow an efficient simulation of statistical models near criticality. This method provides a reliable way to determine c for models, for which the other known methods have failed up to now.

1. Introduction

In our understanding of two-dimensional critical systems the principle of conformal invariance plays a crucial role. It was shown that to each scaling field corresponds a representation of the algebra of the generators of the conformal group, the Virasoro algebra [1]. Particularly important is the central charge c of this algebra, measuring the response of the theory to the curving of the two-dimensional space, the trace anomaly [2,3]. c is an essential quantity in the classification of two-dimensional conformally invariant systems and from this follows the importance of being able to determine the central charge c for statistical models.

A well-known method to determine the central charge c for a given statistical model is based upon finite-size scaling arguments [4]. At the critical point one computes the free energy per site $F(l)$ on an infinitely long strip for increasing values of the width l . The leading finite-size correction to $F(l)$ is related to the central charge and allows a computation of estimates $c(l)$ for c . Of course $c(l)$ converges to the central charge c of the infinite system for $l \rightarrow \infty$. Working in the framework of the transfer matrix or Hamilton formalism, this method was applied successfully to several models [5]. An essential part of this method is the exact diagonalization of the transfer matrix (or hamiltonian) for different values of the width l of the

strip. For many interesting models, however, this exact diagonalization can only be performed in practice for very small values of l , making a reliable extrapolation to the infinite system impossible. Also Monte Carlo simulations are of little help in these difficult cases, because the free energy cannot be measured directly by such simulations. The finite-size scaling method cannot produce any reliable estimates if the manifold in which the statistical variables at each lattice site can take their values is large or even continuous.

Recently Cardy [6] pointed out that the central charge c of the critical system is related to connected correlation functions of the system away from criticality. Such correlation functions can be measured by means of Monte Carlo simulations and we will demonstrate that this relation between c and the connected correlation functions gives rise to an alternative method for the determination of the central charge of the infinite system. The three-state Potts model [7] in a magnetic field was chosen as a test case for several reasons: (i) it is known that $c = 0.8$ for the corresponding field theory [8], (ii) from the computational viewpoint this model is quite challenging, much more so than the Ising model with no magnetic field, for which several methods that break down in more general models are known to work well, (iii) we had developed highly efficient simulation